Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 AM GMT

PDB ID	:	3Q97
Title	:	Crystal structure of human estrogen receptor alpha LBD in complex with GRIP peptide and two isomers of Ethoxy triphenylethylene
Authors	:	Rajan, S.S.; Kim, Y.; Vanek, K.; Joachimiak, A.; Jordan, C.; Greene, G.L.
Deposited on	:	2011-01-07
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

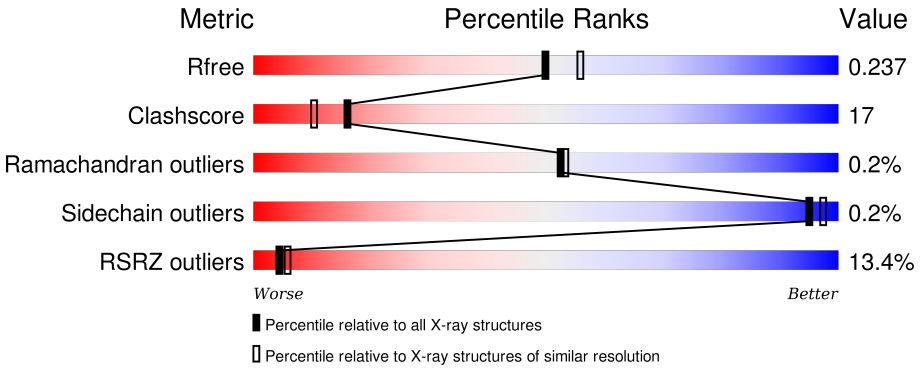
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	8% 77% 18% 5%
2	B	260	15% 76% 17% • 7%
3	C	13	15% 62% 15% 23%
3	D	13	38% 85% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CME	A	381[A]	-	-	X	-
4	Q97	B	600[A]	-	-	X	-
5	SRR	B	601[B]	-	-	X	-
6	FMT	A	1	-	-	-	X
7	GOL	A	2	-	-	X	-
8	CL	A	3	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	16	0
			2051	1312	344	368	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	SER	-	EXPRESSION TAG	UNP P03372
A	296	ASN	-	EXPRESSION TAG	UNP P03372
A	297	ALA	-	EXPRESSION TAG	UNP P03372
A	537	SER	TYR	ENGINEERED MUTATION	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	8	0
			1982	1271	338	352	21			

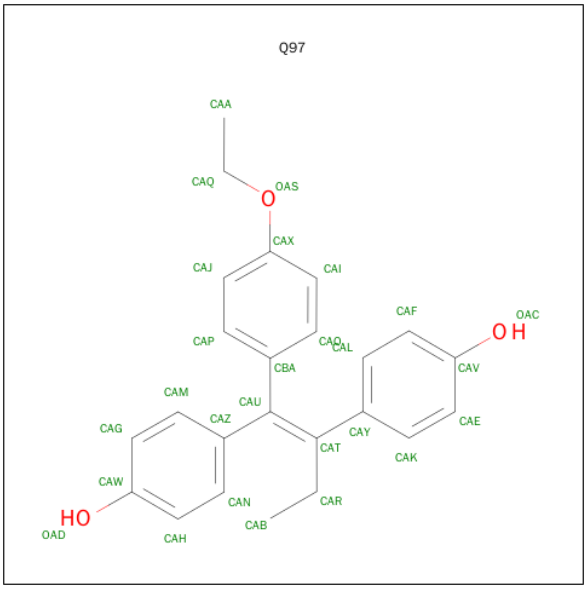
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	295	SER	-	EXPRESSION TAG	UNP P03372
B	296	ASN	-	EXPRESSION TAG	UNP P03372
B	297	ALA	-	EXPRESSION TAG	UNP P03372
B	537	SER	TYR	ENGINEERED MUTATION	UNP P03372

- Molecule 3 is a protein called Estrogen receptor.

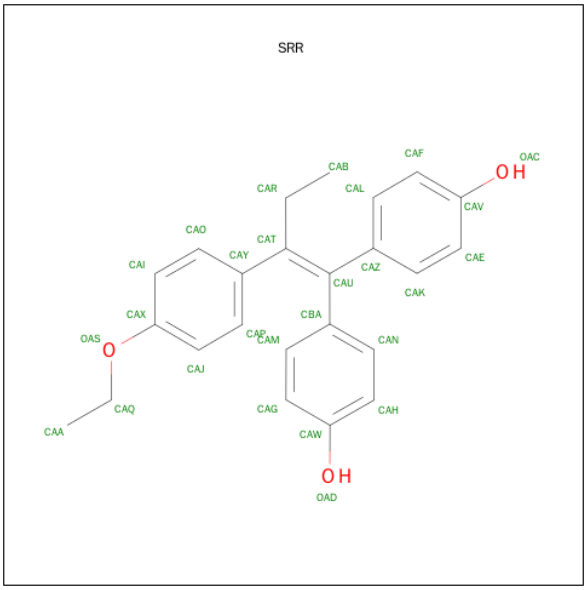
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
3	D	13	Total	C	N	O	0	1	0
			118	74	26	18			

- Molecule 4 is 4,4'-[(1Z)-1-(4-ETHOXYPHENYL)BUT-1-ENE-1,2-DIYL]DIPHENOL (three-letter code: Q97) (formula: $C_{24}H_{24}O_3$).



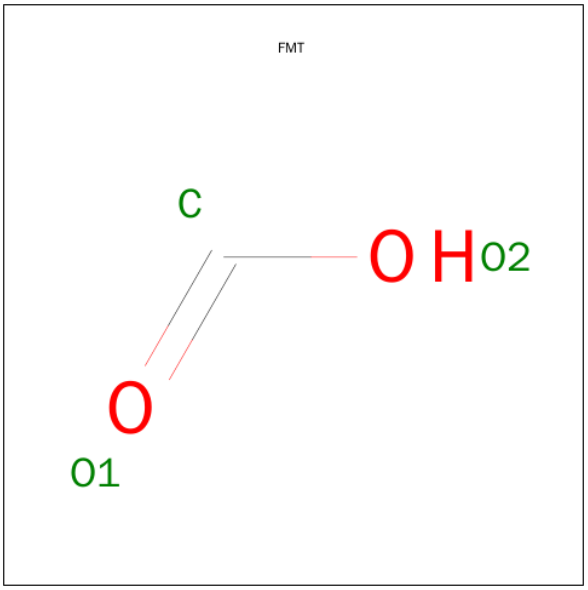
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 27 24 3	0	1
4	B	1	Total C O 27 24 3	0	1

- Molecule 5 is 4,4'-[2-(4-ETHOXYPHENYL)BUT-1-ENE-1,1-DIYL]DIPHENOL (three-letter code: SRR) (formula: $C_{24}H_{24}O_3$).



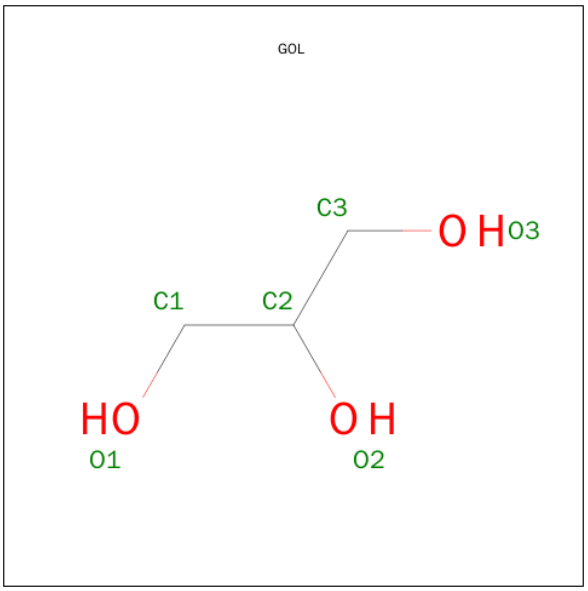
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 27 24 3	0	1
5	B	1	Total C O 27 24 3	0	1

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total Cl 3 3	0	0

- Molecule 9 is water.

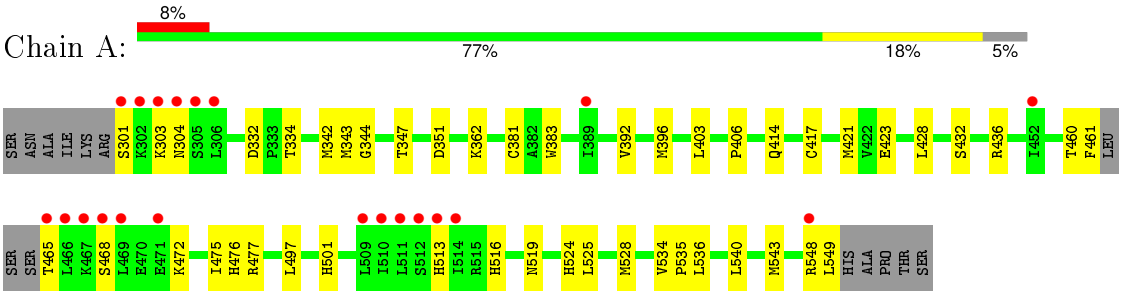
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	59	Total O 59 59	0	0
9	B	33	Total O 33 33	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

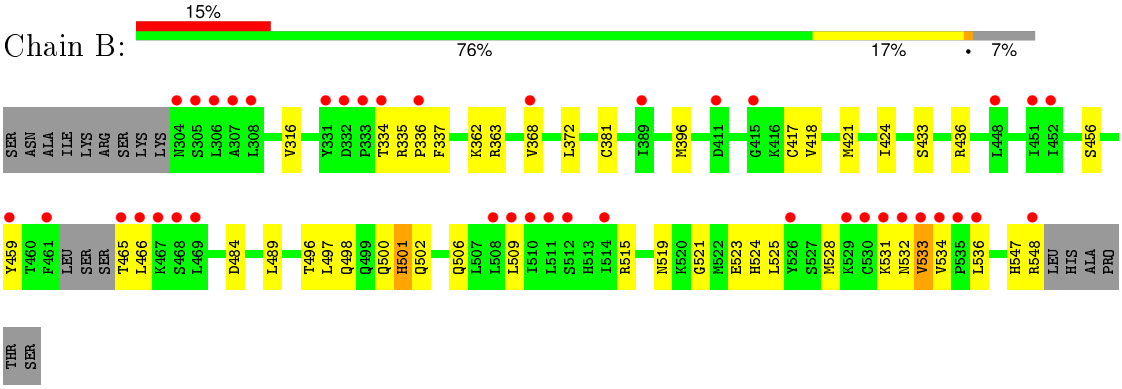
- Molecule 1: Estrogen receptor

Chain A:



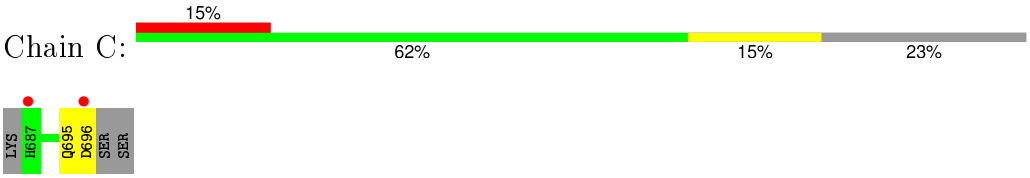
- Molecule 2: Estrogen receptor

Chain B:



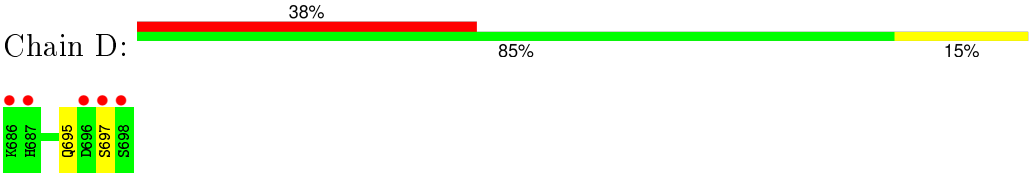
- Molecule 3: Estrogen receptor

Chain C:



- Molecule 3: Estrogen receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.09Å 84.21Å 58.97Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 33.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.10) 93.0 (33.65-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.239 0.199 , 0.237	Depositor DCC
R_{free} test set	1437 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 28284 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, CME, SRR, Q97, FMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/2084	0.54	0/2808
2	B	0.47	0/2022	0.49	0/2728
3	C	0.48	0/90	0.48	0/119
3	D	0.37	0/122	0.45	0/160
All	All	0.48	0/4318	0.51	0/5815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2051	0	2125	75	0
2	B	1982	0	2048	63	0
3	C	89	0	95	3	0
3	D	118	0	131	4	0
4	A	27	0	22	7	0
4	B	27	0	22	15	0
5	A	27	0	22	6	0
5	B	27	0	24	12	0
6	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	8	0
8	A	3	0	0	2	0
9	A	59	0	0	1	0
9	B	33	0	0	2	0
All	All	4452	0	4498	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:600[A]:Q97:CAL	4:B:600[A]:Q97:HAP	1.76	1.15
4:B:600[A]:Q97:HAL	4:B:600[A]:Q97:HAP	1.26	1.14
1:A:519:ASN:HD22	2:B:519:ASN:ND2	1.49	1.09
4:B:600[A]:Q97:CAP	4:B:600[A]:Q97:CAL	2.31	1.07
1:A:519:ASN:ND2	2:B:519:ASN:HD22	1.52	1.06
1:A:417[A]:CME:HB3	1:A:417[A]:CME:HZ3	1.39	1.04
1:A:417[A]:CME:HZ3	1:A:417[A]:CME:CB	1.87	1.03
2:B:363[B]:ARG:NH1	2:B:363[B]:ARG:HG2	1.60	1.01
7:A:2:GOL:H31	2:B:509:LEU:HD12	1.40	1.00
2:B:363[B]:ARG:CG	2:B:363[B]:ARG:HH11	1.75	0.98
1:A:548:ARG:O	1:A:549:LEU:HG	1.65	0.97
2:B:362:LYS:HD3	3:D:697:SER:OG	1.63	0.96
4:B:600[A]:Q97:HARA	4:B:600[A]:Q97:HAM	1.45	0.96
1:A:342[B]:MET:HE3	1:A:342[B]:MET:HA	1.49	0.93
2:B:363[B]:ARG:HG2	2:B:363[B]:ARG:HH11	0.81	0.93
1:A:513[B]:HIS:CD2	2:B:459[B]:TYR:CE2	2.56	0.93
4:B:600[A]:Q97:HARA	4:B:600[A]:Q97:CAM	1.99	0.91
1:A:381[A]:CME:CB	1:A:381[A]:CME:HZ3	2.01	0.91
1:A:342[B]:MET:HA	1:A:342[B]:MET:CE	2.01	0.90
2:B:334:THR:OG1	2:B:335:ARG:NH1	2.03	0.90
1:A:513[B]:HIS:CD2	2:B:459[B]:TYR:CD2	2.61	0.88
2:B:533:VAL:HG13	2:B:534:VAL:H	1.40	0.86
2:B:536:LEU:HD22	4:B:600[A]:Q97:HAAA	1.59	0.84
1:A:381[A]:CME:HB3	1:A:381[A]:CME:HZ3	1.61	0.82
7:A:2:GOL:C3	2:B:509:LEU:HD12	2.09	0.82
1:A:351[B]:ASP:OD1	1:A:540:LEU:HG	1.84	0.76
5:A:601[B]:SRR:CAN	5:A:601[B]:SRR:HAR	2.16	0.75
2:B:465:THR:HG22	2:B:466:LEU:HG	1.69	0.75
2:B:524[B]:HIS:HB3	5:B:601[B]:SRR:HAAB	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381[A]:CME:CA	1:A:381[A]:CME:HZ3	2.20	0.71
5:B:601[B]:SRR:HAR	5:B:601[B]:SRR:HAN	1.72	0.71
2:B:536:LEU:CD2	4:B:600[A]:Q97:HAAA	2.21	0.70
2:B:525:LEU:HD13	4:B:600[A]:Q97:HAQA	1.73	0.70
1:A:428:LEU:HD11	5:A:601[B]:SRR:HAB	1.72	0.70
5:A:601[B]:SRR:HAR	5:A:601[B]:SRR:HAN	1.72	0.69
2:B:524[A]:HIS:HB3	4:B:600[A]:Q97:OAC	1.93	0.69
4:B:600[A]:Q97:CAP	4:B:600[A]:Q97:CAY	2.71	0.68
2:B:533:VAL:HG13	2:B:534:VAL:N	2.08	0.68
1:A:525:LEU:HD13	4:A:600[A]:Q97:HAQA	1.76	0.67
2:B:362:LYS:CD	3:D:697:SER:OG	2.42	0.67
1:A:423:GLU:HB2	8:A:3:CL:CL	2.32	0.66
1:A:342[B]:MET:CA	1:A:342[B]:MET:CE	2.74	0.66
3:C:695:GLN:O	3:C:696:ASP:HB3	1.97	0.65
1:A:465:THR:HA	1:A:468:SER:OG	1.97	0.65
2:B:524[A]:HIS:CE1	2:B:528:MET:CE	2.79	0.64
2:B:337:PHE:HB2	2:B:417:CME:HE3	1.80	0.63
1:A:343:MET:SD	1:A:528:MET:HE1	2.39	0.63
1:A:428:LEU:CD1	5:A:601[B]:SRR:HAB	2.28	0.62
2:B:525:LEU:HD21	4:B:600[A]:Q97:CAJ	2.29	0.62
2:B:524[A]:HIS:CE1	2:B:528:MET:HE1	2.34	0.62
2:B:372:LEU:CD2	3:D:695:GLN:HE21	2.11	0.62
1:A:421:MET:SD	5:A:601[B]:SRR:HAJ	2.40	0.61
5:B:601[B]:SRR:HAP	5:B:601[B]:SRR:HABB	1.81	0.61
1:A:381[A]:CME:HB3	1:A:381[A]:CME:CZ	2.28	0.61
1:A:383:TRP:CD1	1:A:543:MET:CE	2.83	0.61
1:A:513[B]:HIS:CG	2:B:459[B]:TYR:CD2	2.88	0.61
5:B:601[B]:SRR:CAN	5:B:601[B]:SRR:CAR	2.80	0.60
1:A:362:LYS:NZ	3:C:696:ASP:OD1	2.34	0.60
5:B:601[B]:SRR:CAP	5:B:601[B]:SRR:CAB	2.80	0.59
1:A:461:PHE:HE2	1:A:475:ILE:HD12	1.66	0.59
1:A:381[A]:CME:HZ3	1:A:381[A]:CME:HA	1.84	0.58
2:B:524[B]:HIS:CB	5:B:601[B]:SRR:HAAB	2.33	0.58
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.85	0.58
2:B:547:HIS:O	2:B:548:ARG:C	2.42	0.58
2:B:368[A]:VAL:HG22	9:B:2:HOH:O	2.04	0.57
1:A:461:PHE:CE2	1:A:475:ILE:HD12	2.40	0.56
1:A:513[B]:HIS:CD2	2:B:459[B]:TYR:HE2	2.19	0.56
4:A:600[A]:Q97:HAM	4:A:600[A]:Q97:CAR	2.36	0.56
4:A:600[A]:Q97:HARA	4:A:600[A]:Q97:CAM	2.36	0.55
1:A:417[A]:CME:HB3	1:A:417[A]:CME:CZ	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524[B]:HIS:CG	5:B:601[B]:SRR:HAAB	2.42	0.55
1:A:548:ARG:O	1:A:549:LEU:CG	2.49	0.55
1:A:461:PHE:HD2	1:A:472:LYS:HG3	1.72	0.54
4:B:600[A]:Q97:HAM	4:B:600[A]:Q97:CAR	2.25	0.54
1:A:524[B]:HIS:HB3	5:A:601[B]:SRR:HAAA	1.89	0.54
4:A:600[A]:Q97:CAM	4:A:600[A]:Q97:CAR	2.84	0.54
2:B:524[A]:HIS:CE1	2:B:528:MET:HE2	2.42	0.54
1:A:383:TRP:CD1	1:A:543:MET:HE3	2.43	0.54
2:B:531:LYS:O	2:B:532:ASN:HB2	2.07	0.54
1:A:343:MET:CE	1:A:528:MET:HE3	2.38	0.54
3:C:695:GLN:O	3:C:696:ASP:CB	2.55	0.54
2:B:521:GLY:CA	4:B:600[A]:Q97:HAE	2.37	0.54
1:A:417[B]:CME:HB2	1:A:417[B]:CME:OH	2.07	0.54
2:B:533:VAL:CG1	2:B:534:VAL:H	2.17	0.54
5:B:601[B]:SRR:CAP	5:B:601[B]:SRR:HABB	2.38	0.54
1:A:524[A]:HIS:ND1	4:A:600[A]:Q97:OAC	2.37	0.53
5:B:601[B]:SRR:HAN	5:B:601[B]:SRR:CAR	2.36	0.53
7:A:2:GOL:H2	2:B:506:GLN:HA	1.90	0.53
1:A:342[B]:MET:HE2	1:A:342[B]:MET:HA	1.88	0.53
1:A:513[B]:HIS:CG	2:B:459[B]:TYR:CE2	2.96	0.52
1:A:417[A]:CME:HZ3	1:A:417[A]:CME:CA	2.39	0.52
1:A:476:HIS:HD2	7:A:2:GOL:O1	1.93	0.52
4:A:600[A]:Q97:CAY	4:A:600[A]:Q97:CAP	2.88	0.52
4:B:600[A]:Q97:CAM	4:B:600[A]:Q97:CAR	2.76	0.51
1:A:301:SER:HA	1:A:304:ASN:OD1	2.12	0.50
2:B:496:THR:O	2:B:500:GLN:HG3	2.11	0.50
1:A:392:VAL:HG13	1:A:432[A]:SER:HA	1.92	0.50
7:A:2:GOL:C3	2:B:509:LEU:CD1	2.88	0.49
2:B:335:ARG:HB3	2:B:336:PRO:HD2	1.95	0.49
1:A:392:VAL:HG13	1:A:432[B]:SER:HA	1.94	0.49
1:A:476:HIS:CD2	7:A:2:GOL:O1	2.66	0.48
1:A:347[B]:THR:HG21	1:A:536:LEU:CD2	2.42	0.48
2:B:418:VAL:HB	2:B:421:MET:HE2	1.96	0.48
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.43	0.48
2:B:501[A]:HIS:CD2	2:B:502:GLN:N	2.82	0.48
2:B:523:GLU:OE1	9:B:79:HOH:O	2.20	0.47
7:A:2:GOL:H31	2:B:509:LEU:CD1	2.29	0.47
7:A:2:GOL:H2	2:B:506:GLN:CG	2.45	0.47
2:B:396:MET:CE	2:B:436:ARG:HA	2.44	0.47
1:A:383:TRP:CG	1:A:543:MET:HE2	2.50	0.47
2:B:533:VAL:CG1	2:B:534:VAL:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:456:SER:HA	2:B:515:ARG:NH2	2.30	0.46
2:B:381:CME:SG	2:B:381:CME:OH	2.71	0.46
1:A:383:TRP:CD1	1:A:543:MET:HE2	2.49	0.46
1:A:392:VAL:HG13	1:A:432[B]:SER:CA	2.45	0.46
2:B:316:VAL:HG21	2:B:489:LEU:HD21	1.98	0.46
5:B:601[B]:SRR:HAJ	5:B:601[B]:SRR:HAQ	1.68	0.45
1:A:301:SER:O	1:A:304:ASN:ND2	2.50	0.45
1:A:332:ASP:OD1	1:A:334:THR:OG1	2.34	0.45
1:A:461:PHE:HD2	1:A:472:LYS:CG	2.30	0.45
1:A:303:LYS:HG3	1:A:477:ARG:HH22	1.82	0.44
1:A:414:GLN:O	1:A:417[B]:CME:SG	2.76	0.44
1:A:347[B]:THR:HG23	1:A:540:LEU:CD1	2.48	0.44
2:B:521:GLY:HA3	4:B:600[A]:Q97:HAE	1.99	0.44
2:B:424:ILE:HD11	2:B:524[B]:HIS:HD2	1.83	0.44
2:B:433[B]:SER:OG	2:B:436:ARG:NH2	2.51	0.44
1:A:516:HIS:HA	2:B:519:ASN:HD21	1.83	0.43
1:A:513[B]:HIS:CD2	2:B:459[B]:TYR:HD2	2.29	0.43
2:B:424:ILE:HD11	2:B:524[B]:HIS:CD2	2.53	0.43
1:A:525:LEU:HD21	4:A:600[A]:Q97:CAJ	2.48	0.43
2:B:372:LEU:HD22	3:D:695:GLN:HE21	1.80	0.43
1:A:501[B]:HIS:HE1	2:B:484:ASP:OD1	2.01	0.43
5:B:601[B]:SRR:HAR	5:B:601[B]:SRR:CAN	2.42	0.43
1:A:342[B]:MET:CA	1:A:342[B]:MET:HE2	2.48	0.42
1:A:392:VAL:HG13	1:A:432[A]:SER:CA	2.46	0.42
1:A:497:LEU:HD21	2:B:497:LEU:HD21	1.99	0.42
1:A:396:MET:HE2	1:A:436:ARG:HA	2.01	0.42
1:A:344:GLY:HA2	1:A:534:VAL:HG21	2.02	0.42
1:A:460:THR:HG23	9:A:87:HOH:O	2.19	0.42
1:A:343:MET:CE	1:A:528:MET:CE	2.97	0.42
2:B:498:GLN:O	2:B:502:GLN:HG3	2.19	0.42
1:A:513[B]:HIS:NE2	2:B:459[B]:TYR:HD2	2.18	0.42
1:A:381[A]:CME:CB	1:A:381[A]:CME:CZ	2.86	0.42
1:A:403[B]:LEU:HD11	1:A:406:PRO:HA	2.02	0.41
2:B:528:MET:HE2	5:B:601[B]:SRR:HAQA	2.03	0.41
1:A:423:GLU:CB	8:A:3:CL:CL	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	253/260 (97%)	251 (99%)	2 (1%)	0	100 100
2	B	244/260 (94%)	241 (99%)	2 (1%)	1 (0%)	39 37
3	C	8/13 (62%)	8 (100%)	0	0	100 100
3	D	12/13 (92%)	10 (83%)	2 (17%)	0	100 100
All	All	517/546 (95%)	510 (99%)	6 (1%)	1 (0%)	52 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	533	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	233/231 (101%)	233 (100%)	0	100 100
2	B	224/232 (97%)	222 (99%)	2 (1%)	84 89
3	C	10/13 (77%)	10 (100%)	0	100 100
3	D	14/13 (108%)	14 (100%)	0	100 100
All	All	481/489 (98%)	479 (100%)	2 (0%)	95 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	501[A]	HIS
2	B	501[B]	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	HIS
1	A	476	HIS
2	B	498	GLN
2	B	519	ASN
3	D	695	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CME	A	381[A]	-	8,9,10	0.77	0	6,9,11	2.70	1 (16%)
1	CME	A	381[B]	-	8,9,10	0.69	0	6,9,11	2.34	1 (16%)
1	CME	A	417[A]	1	8,9,10	0.80	0	6,9,11	2.24	1 (16%)
1	CME	A	417[B]	1	8,9,10	0.76	0	6,9,11	1.51	2 (33%)
1	CME	A	530	1	8,9,10	0.74	0	6,9,11	2.07	3 (50%)
2	CME	B	381	2	8,9,10	0.64	0	6,9,11	2.77	2 (33%)
2	CME	B	417	2	8,9,10	0.66	0	6,9,11	2.62	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	381[A]	-	-	0/5/8/10	0/0/0/0
1	CME	A	381[B]	-	-	0/5/8/10	0/0/0/0
1	CME	A	417[A]	1	-	0/5/8/10	0/0/0/0
1	CME	A	417[B]	1	-	0/5/8/10	0/0/0/0
1	CME	A	530	1	-	0/5/8/10	0/0/0/0
2	CME	B	381	2	-	0/5/8/10	0/0/0/0
2	CME	B	417	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	CME	CZ-CE-SD	-2.35	107.42	113.16
1	A	417[B]	CME	O-C-CA	-2.13	119.95	125.49
1	A	530	CME	O-C-CA	-2.08	120.08	125.49
2	B	381	CME	O-C-CA	-2.05	120.14	125.49
1	A	417[B]	CME	CB-SG-SD	2.79	109.38	103.95
1	A	530	CME	CB-SG-SD	3.48	110.74	103.95
1	A	417[A]	CME	CB-SG-SD	4.88	113.46	103.95
1	A	381[B]	CME	CB-SG-SD	5.00	113.70	103.95
2	B	381	CME	CB-SG-SD	5.88	115.42	103.95
2	B	417	CME	CB-SG-SD	5.97	115.58	103.95
1	A	381[A]	CME	CB-SG-SD	6.09	115.83	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381[A]	CME	6	0
1	A	417[A]	CME	4	0
1	A	417[B]	CME	2	0
2	B	381	CME	1	0
2	B	417	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FMT	A	1	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	A	2	-	5,5,5	0.32	0	5,5,5	0.65	0
4	Q97	A	600[A]	-	29,29,29	1.83	3 (10%)	39,39,39	1.40	6 (15%)
5	SRR	A	601[B]	-	29,29,29	1.77	3 (10%)	39,39,39	1.15	2 (5%)
4	Q97	B	600[A]	-	29,29,29	1.83	3 (10%)	39,39,39	1.72	5 (12%)
5	SRR	B	601[B]	-	29,29,29	1.66	3 (10%)	39,39,39	1.04	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FMT	A	1	-	-	0/0/0/0	0/0/0/0
7	GOL	A	2	-	-	0/4/4/4	0/0/0/0
4	Q97	A	600[A]	-	-	0/21/21/21	0/3/3/3
5	SRR	A	601[B]	-	-	0/21/21/21	0/3/3/3
4	Q97	B	600[A]	-	-	0/21/21/21	0/3/3/3
5	SRR	B	601[B]	-	-	0/21/21/21	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600[A]	Q97	CAZ-CAU	-5.85	1.39	1.49
4	A	600[A]	Q97	CAZ-CAU	-5.78	1.39	1.49
4	B	600[A]	Q97	CBA-CAU	-5.66	1.39	1.49
4	A	600[A]	Q97	CBA-CAU	-5.46	1.40	1.49
5	B	601[B]	SRR	CAZ-CAU	-5.40	1.40	1.49
5	A	601[B]	SRR	CAZ-CAU	-5.36	1.40	1.49
5	A	601[B]	SRR	CBA-CAU	-5.35	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600[A]	Q97	CAY-CAT	-5.15	1.38	1.49
5	A	601[B]	SRR	CAY-CAT	-5.01	1.39	1.49
4	B	600[A]	Q97	CAY-CAT	-4.98	1.39	1.49
5	B	601[B]	SRR	CBA-CAU	-4.88	1.41	1.49
5	B	601[B]	SRR	CAY-CAT	-4.22	1.40	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	600[A]	Q97	CAY-CAT-CAU	-6.31	114.24	122.40
4	A	600[A]	Q97	CAY-CAT-CAU	-4.39	116.73	122.40
5	A	601[B]	SRR	CAQ-OAS-CAX	-3.80	110.25	117.92
4	A	600[A]	Q97	CAK-CAY-CAT	-3.79	115.44	120.99
4	B	600[A]	Q97	CAQ-OAS-CAX	-3.30	111.26	117.92
5	B	601[B]	SRR	CAR-CAT-CAU	-3.28	119.74	123.47
5	A	601[B]	SRR	CAK-CAZ-CAU	-3.23	116.21	120.92
4	B	600[A]	Q97	CBA-CAU-CAT	-3.23	118.51	122.84
5	B	601[B]	SRR	CAQ-OAS-CAX	-2.89	112.08	117.92
4	A	600[A]	Q97	CAQ-OAS-CAX	-2.44	113.00	117.92
4	A	600[A]	Q97	CBA-CAU-CAT	-2.00	120.15	122.84
4	A	600[A]	Q97	CAL-CAY-CAT	2.31	124.37	120.99
4	B	600[A]	Q97	CBA-CAU-CAZ	2.52	120.88	115.69
5	B	601[B]	SRR	CAR-CAT-CAY	3.54	119.54	114.39
4	A	600[A]	Q97	CAR-CAT-CAY	3.79	119.89	114.39
4	B	600[A]	Q97	CAR-CAT-CAY	5.49	122.36	114.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2	GOL	8	0
4	A	600[A]	Q97	7	0
5	A	601[B]	SRR	6	0
4	B	600[A]	Q97	15	0
5	B	601[B]	SRR	12	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	243/260 (93%)	0.37	21 (8%) 13 18	19, 34, 73, 118	4 (1%)
2	B	240/260 (92%)	0.75	40 (16%) 2 3	22, 41, 103, 145	0
3	C	10/13 (76%)	0.16	2 (20%) 1 2	30, 43, 69, 72	0
3	D	13/13 (100%)	1.50	5 (38%) 0 0	41, 63, 97, 101	0
All	All	506/546 (92%)	0.58	68 (13%) 4 6	19, 37, 92, 145	4 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	333	PRO	7.8
2	B	465	THR	6.7
1	A	465	THR	6.2
2	B	531	LYS	5.5
3	D	686	LYS	5.5
2	B	533	VAL	5.2
1	A	468	SER	5.1
2	B	530	CYS	4.8
1	A	303	LYS	4.7
1	A	305	SER	4.5
2	B	334	THR	4.3
1	A	548	ARG	4.2
2	B	459[A]	TYR	4.1
2	B	534	VAL	4.0
1	A	467	LYS	4.0
2	B	306	LEU	3.9
2	B	511	LEU	3.9
1	A	301	SER	3.8
2	B	304	ASN	3.8
3	C	696	ASP	3.7
2	B	532	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	468	SER	3.6
2	B	305	SER	3.6
3	D	696	ASP	3.4
1	A	306	LEU	3.4
2	B	526	TYR	3.4
2	B	308	LEU	3.4
2	B	461	PHE	3.3
2	B	508	LEU	3.3
2	B	415	GLY	3.2
2	B	452	ILE	3.2
2	B	466	LEU	3.2
2	B	389	ILE	3.2
1	A	302	LYS	3.2
1	A	469	LEU	3.2
2	B	469	LEU	3.2
3	D	698	SER	3.1
1	A	511	LEU	3.1
1	A	452	ILE	3.1
1	A	512[A]	SER	3.1
2	B	509	LEU	3.0
1	A	514	ILE	3.0
2	B	514	ILE	2.9
2	B	548	ARG	2.9
3	D	687	HIS	2.9
1	A	389	ILE	2.9
1	A	471	GLU	2.8
1	A	304	ASN	2.8
2	B	448	LEU	2.7
2	B	368[A]	VAL	2.6
1	A	510	ILE	2.6
2	B	512	SER	2.6
2	B	307	ALA	2.6
2	B	529	LYS	2.6
2	B	451	ILE	2.6
1	A	466	LEU	2.5
2	B	510	ILE	2.5
2	B	336	PRO	2.4
2	B	535	PRO	2.4
2	B	411	ASP	2.4
2	B	331	TYR	2.2
2	B	536	LEU	2.2
2	B	467	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	509	LEU	2.2
3	C	687	HIS	2.2
3	D	697	SER	2.1
2	B	332	ASP	2.1
1	A	513[A]	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CME	A	381[A]	10/11	0.97	0.13	-	22,23,37,38	7
1	CME	A	530	10/11	0.95	0.21	-	41,45,62,64	0
2	CME	B	417	10/11	0.86	0.23	-	68,70,80,81	5
1	CME	A	417[A]	10/11	0.90	0.19	-	44,46,59,61	10
1	CME	A	417[B]	10/11	0.90	0.19	-	45,47,62,63	10
2	CME	B	381	10/11	0.92	0.12	-	29,32,63,65	0
1	CME	A	381[B]	10/11	0.97	0.13	-	22,23,37,40	7

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	FMT	A	1	3/3	0.86	0.36	2.95	41,41,41,43	0
7	GOL	A	2	6/6	0.90	0.19	0.90	44,47,49,50	0
8	CL	A	4	1/1	0.84	0.14	0.52	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SRR	A	601[B]	27/27	0.95	0.13	-0.21	30,34,49,50	27
4	Q97	B	600[A]	27/27	0.95	0.14	-0.25	19,25,27,29	27
4	Q97	A	600[A]	27/27	0.96	0.12	-0.32	23,27,30,31	27
5	SRR	B	601[B]	27/27	0.94	0.12	-0.85	32,42,45,47	27
8	CL	A	3	1/1	0.97	0.15	-	66,66,66,66	0
8	CL	A	5	1/1	0.94	0.19	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.